Python at Warp Speed

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Introduction

Scientist,
Head of department

Deutsches Zentrum
für Luft- und Raumfahrt
German Aerospace Center

Co-Founder, Data
Scientist, and Patient

medando

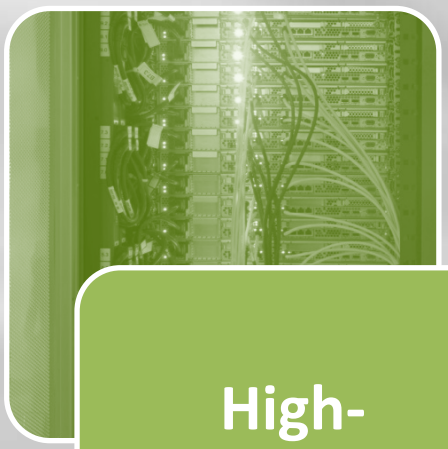
Communities

Quantified Self
Meetup Cologne

cologne

PyHPC2016

Python at Warp Speed



High-Performance Computing

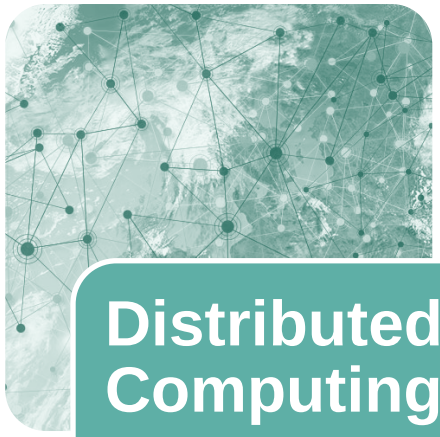
Distributed Computing

Quantum Computing

Algorithmic View
Input x – Algorithm $\boxed{A}$ – Output y

High-Perf. Computing

- □
  Compute



Distributed Computing

- □
  Learn

Quantum Computing

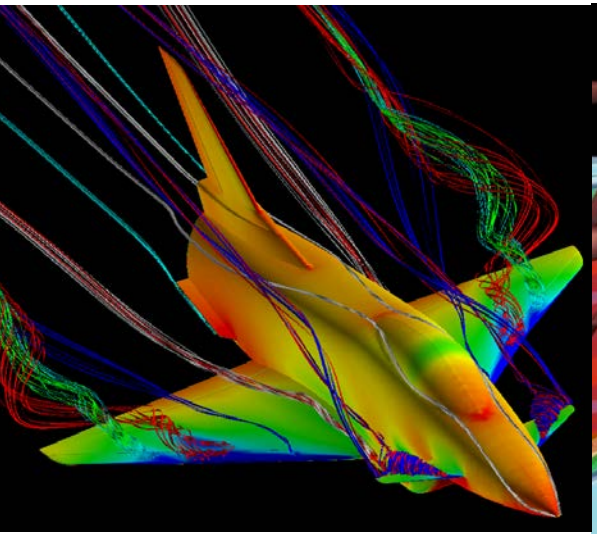
- □
  Optimize

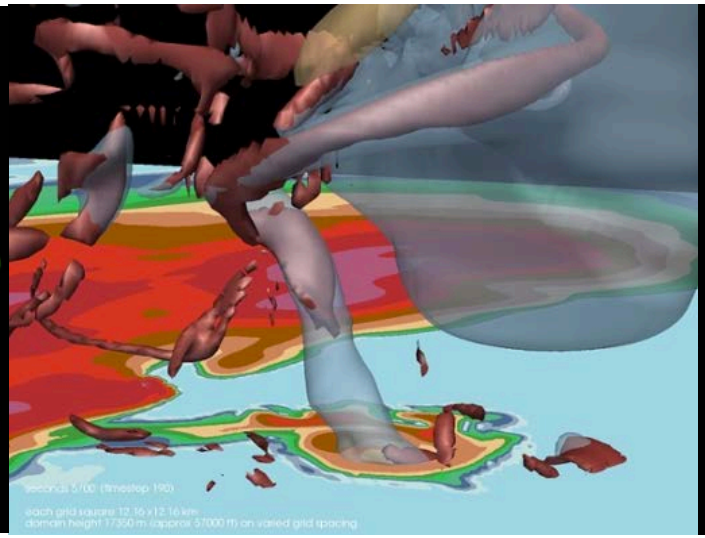
High-Performance Computing

High-Performance Computing

High raw computing power for large science applications

- Huge performance on a single / multi-core processors
- Huge machines with up to millions of cores





Images: DLR & https://sciencenode.org

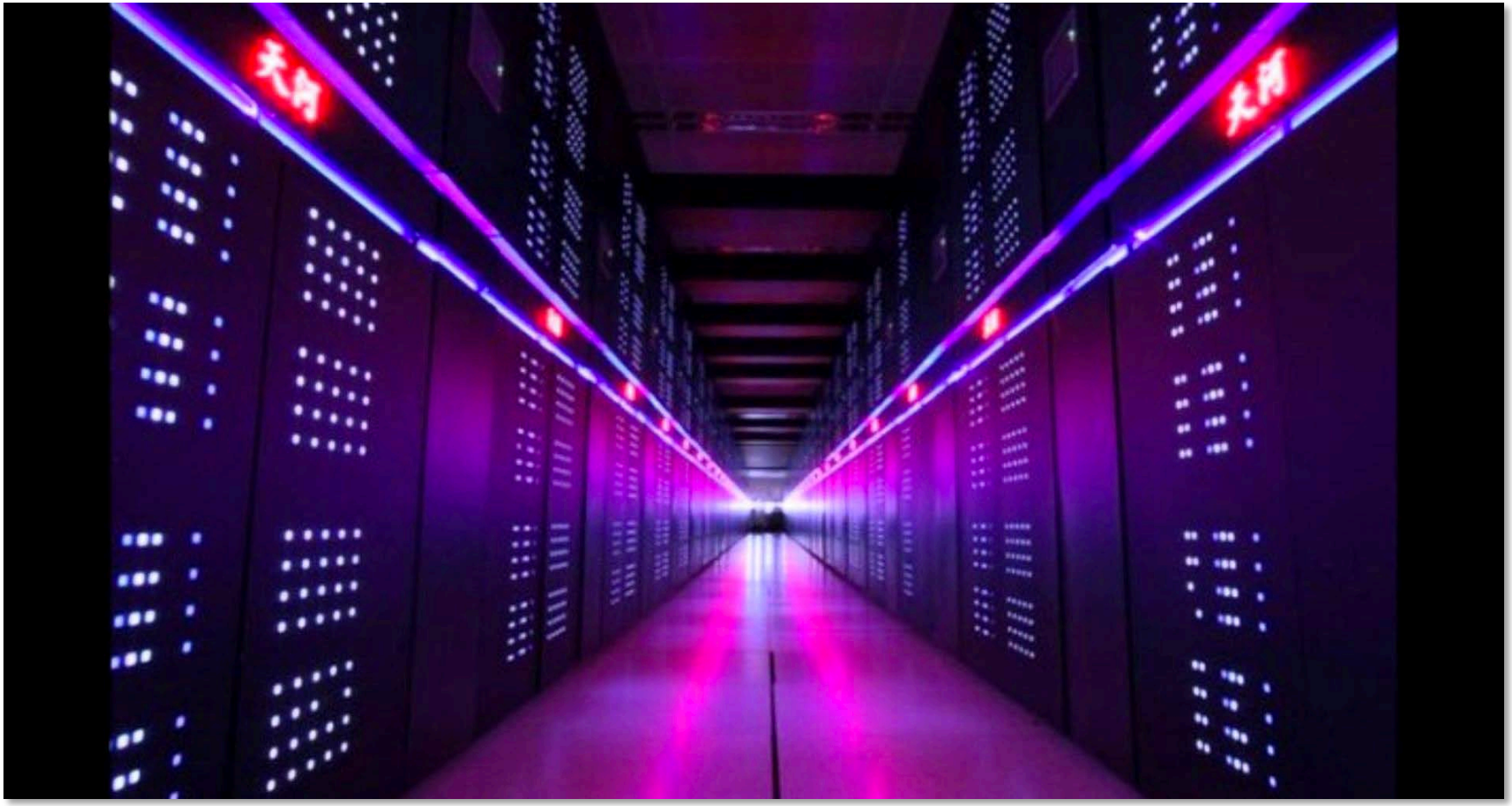
Sunway TaihuLight

10.649.600 Cores, 93 PetaFLOPS

DLR

Tianhe-2 (天河二号)

3.120.000 Cores, 33,8 PetaFLOPS



DLR

Titan

560.640 Cores, 17,5 PetaFLOPS

DLR

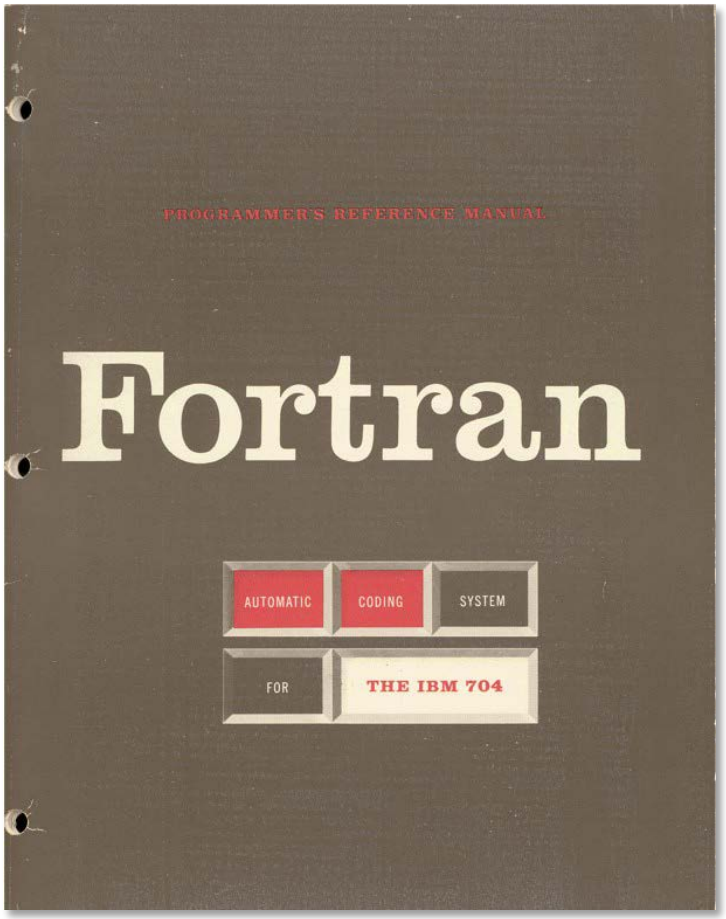
Programming HPC

Technologies

- MPI (Message Passing Interface)
- OpenMP (Open Multi-Processing)
- OpenACC (Open Accelerators)
- Global Arrays Toolkit
- CUDA (GPGPUs)
- OpenCL (GPGPUs)

Languages

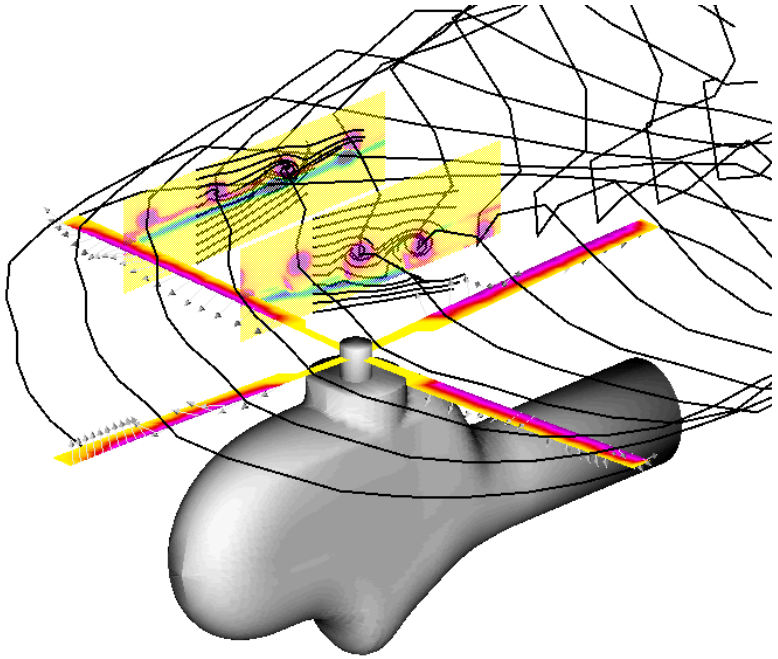
- Fortran
- Fortran
- C/C++
- **Python**



Performance Fortran vs. Python
Helicopter Simulation

Fortran Code

- Developed 1994-1996
- parallelized with MPI
- Performance optimization 2013/14 with MPI und OpenACC



Performance Comparison

- Multi-core CPUs
  - Cython mit OpenMP
  - Python bindings for Global Array Toolkit
- GPGPUs
  - NumbaPro

Core Computation Loops in Pure Python

```
for iblades in range(numberOfBlades):
    for iradial in range(1, dimensionInRadialDirection):
        for iazimutal in range(dimensionInAzimualDirectionTotal):
            for i1 in range(len(vx[0])):
                for i2 in range(len(vx[0][0])):
                    for i3 in range(len(vx[0][0][0])):
                        # wilin-Aufruf 1
for iblades in range(numberOfBlades):
    for iradial in range(dimensionInRadialDirection):
        for iazimutal in range(1, dimensionInAzimualDirectionTotal):
            for i1 in range(len(vx[0])):
                for i2 in range(len(vx[0][0])):
                    for i3 in range(len(vx[0][0][0])):
                        # wilin-Aufruf 2
for iDir in range(3):
    for i in range(numberOfBlades):
        for j in range(dimensionInRadialDirection):
            for k in range(dimensionInAzimualDirectionTotal):
                 x[iDir][i][j][k] = x[iDir][i][j][k] +
                                    dt * vx[iDir][i][j][k]
```

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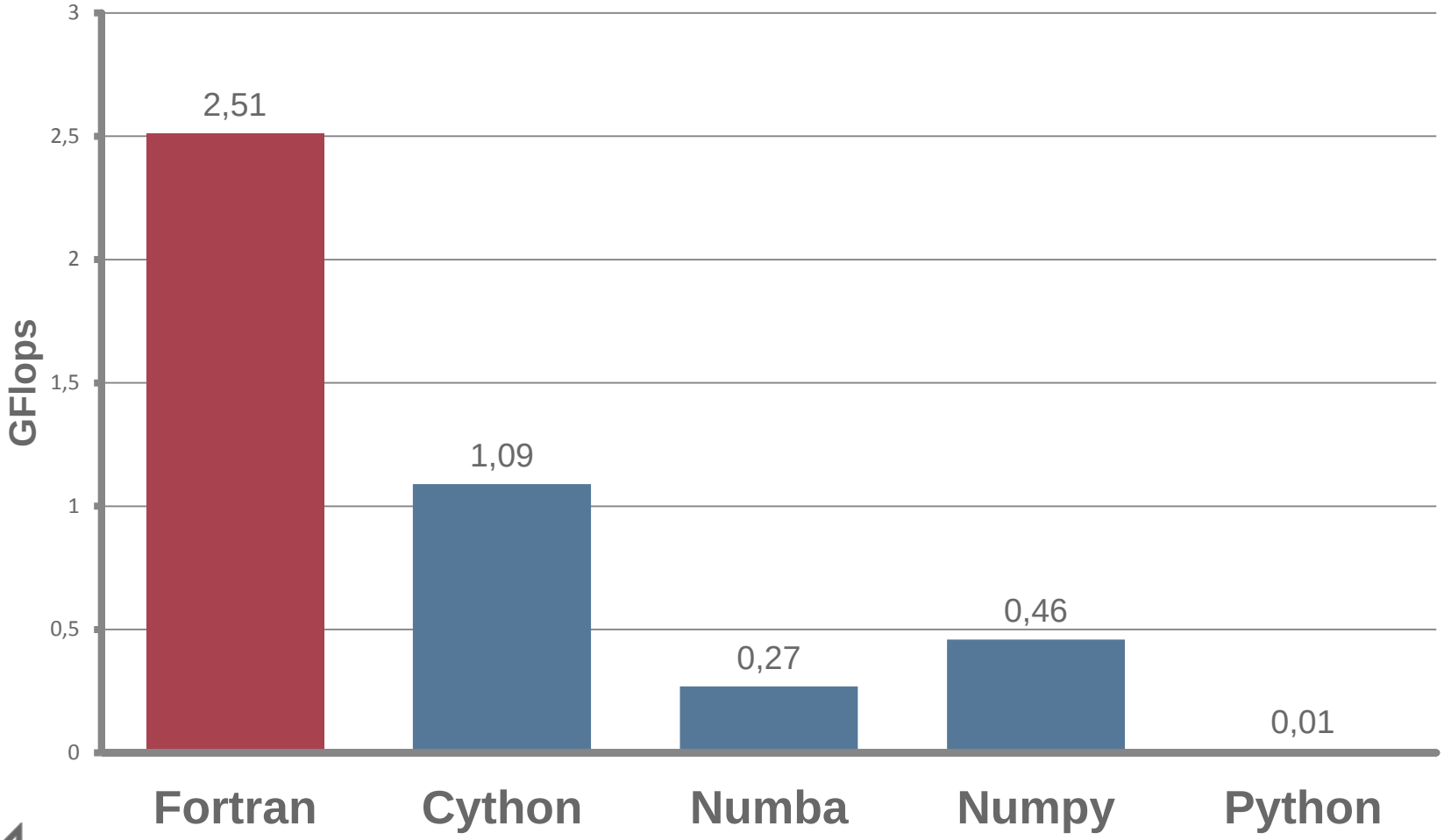
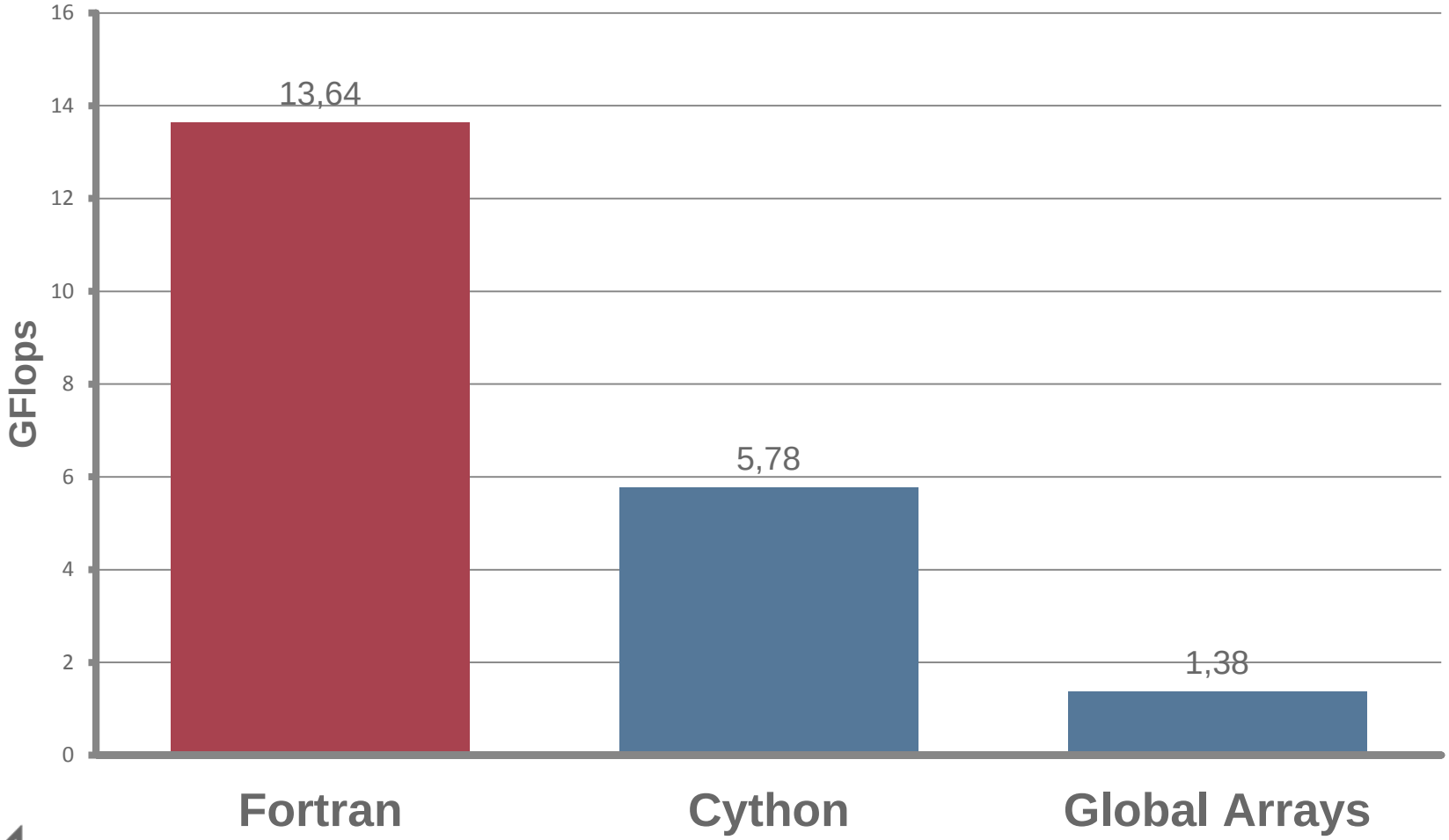
Performance Fortran vs. Python

Single Core (Xeon E5645, 6 Cores)



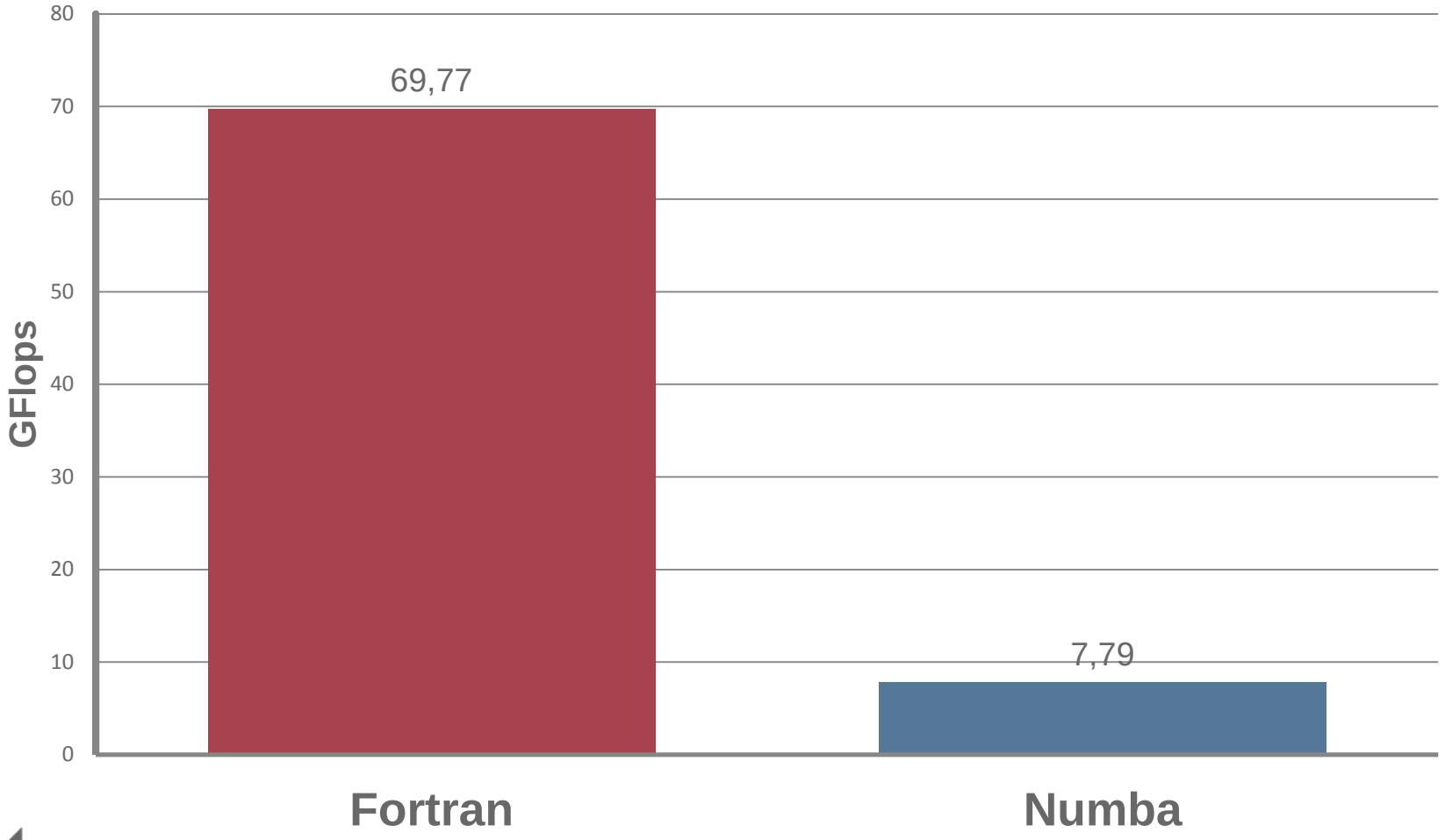
Performance Fortran vs. Python

Multi-Core (Xeon E5645, 6 Cores)

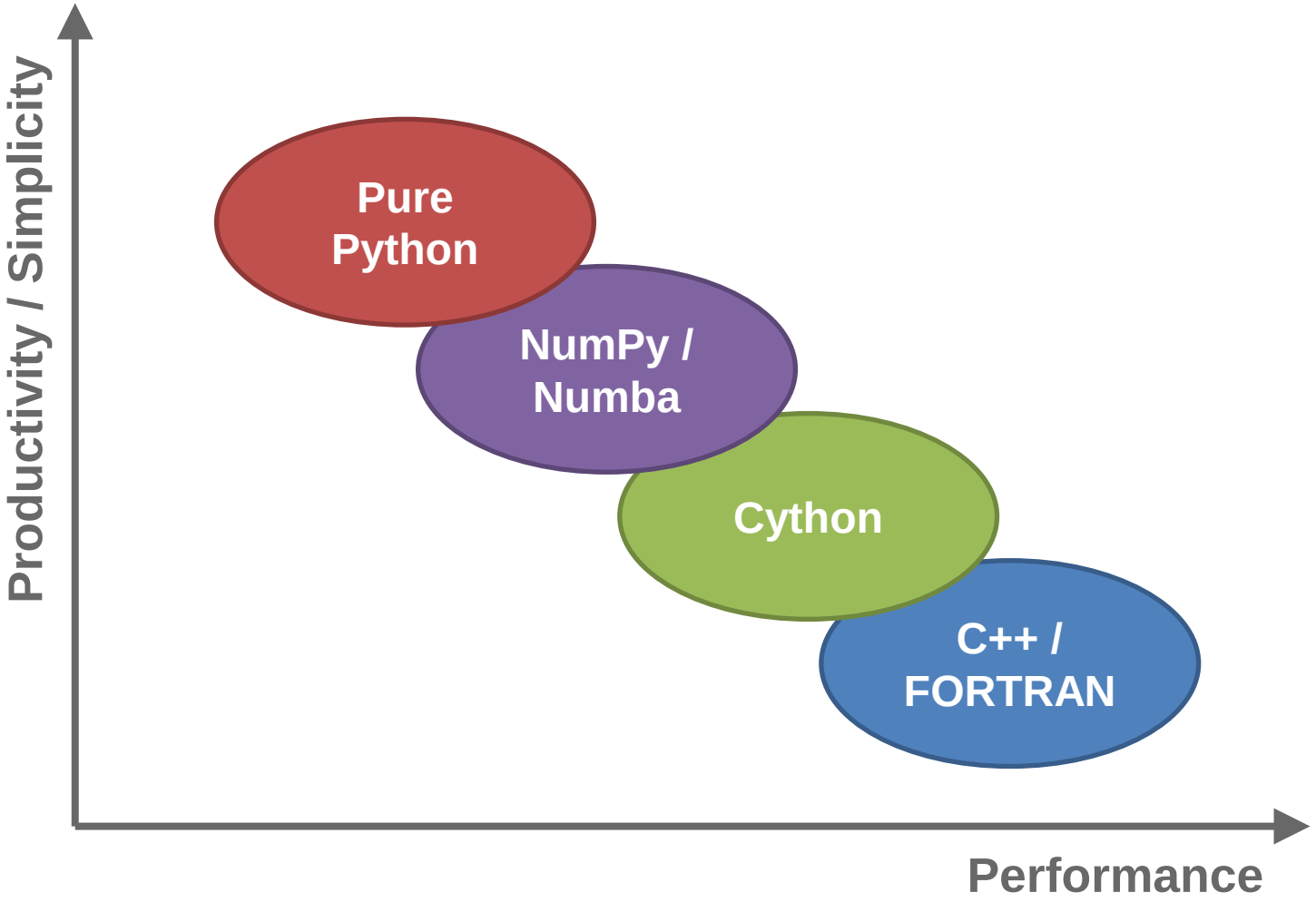


Performance Fortran vs. Python

GPGPU (NVIDIA Tesla C2075, 448 CUDA-Cores)



Performance-Productivity-Space



Productivity vs. Performance of Python

Python's productivity is great

- Allows to write code quickly
- Wide range of applications

Python's performance still needs improvements

- Code optimization with tools for profiling, code examination, …
- Optimized libraries for parallel processing with MPI etc.

Excited to see advancements by community and companies

Workshop „Python for High-Performance and Scientific Computing“ (PyHPC)

Annual scientific workshop, in conjunction with Supercomputing conference

SC16
Salt Lake City, Utah | hpc matters.

State-of-the-art in

- Hybrid programming
- Comparison with other languages for HPC
- Interactive parallel computing
- High-performance computing applications
- Performance analysis, profiling, and debugging

PyHPC 2016

- 6th edition, Nov 14, 2016, Salt Lake City
- `http://www.dlr.de/sc/pyhpc2016`

PyHPC2016

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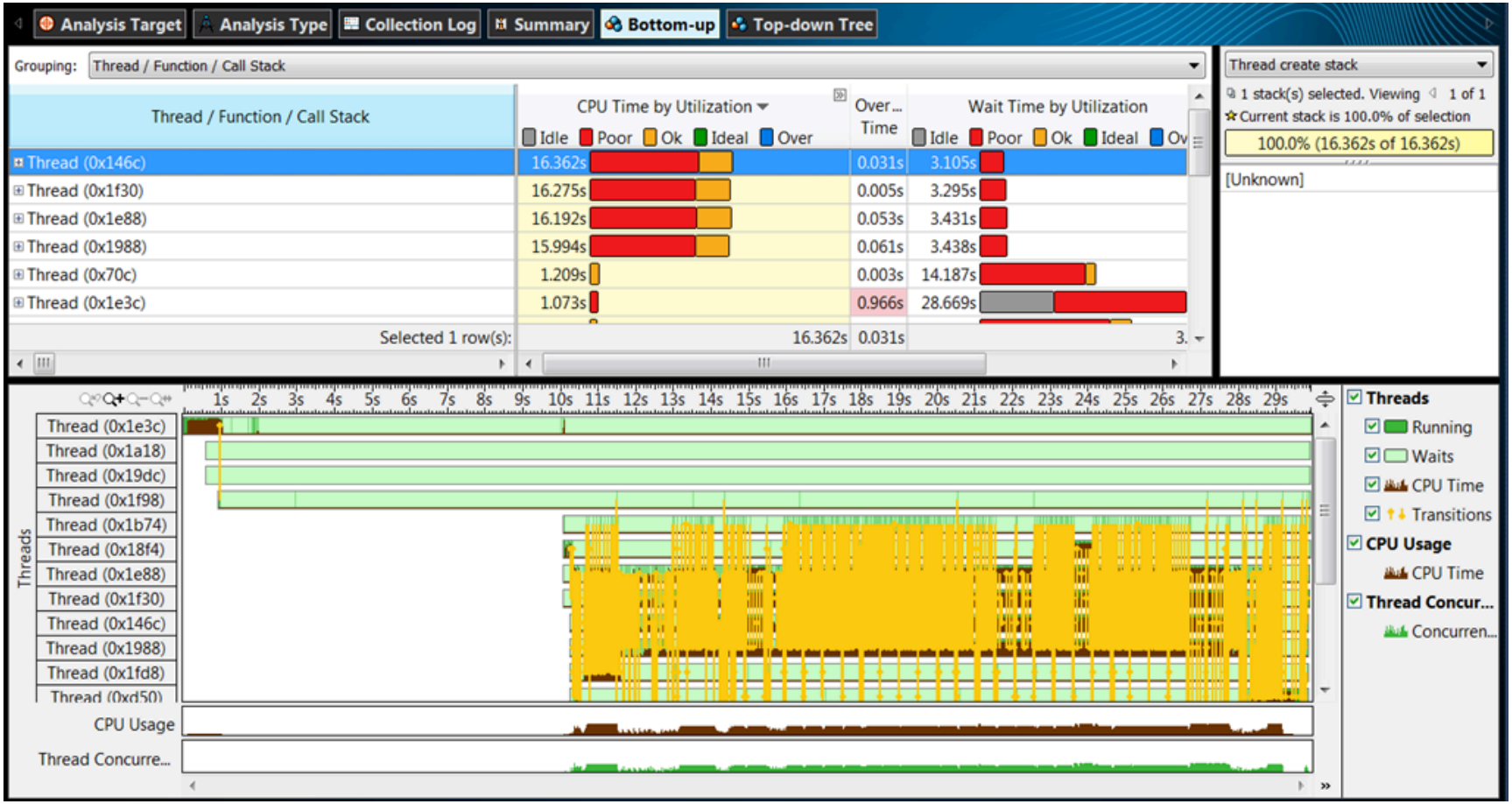
Tools Example

Intel® VTune™ Amplifier for Profiling

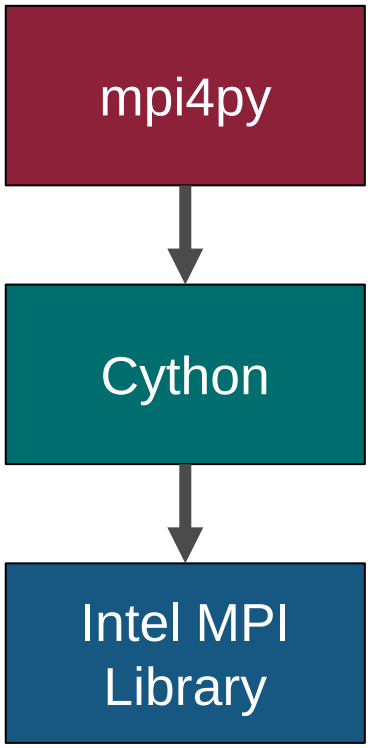


https://software.intel.com/en-us/intel-vtune-amplifier-xe/

Tools Example

mpi4py with Intel MPI Library and Cython

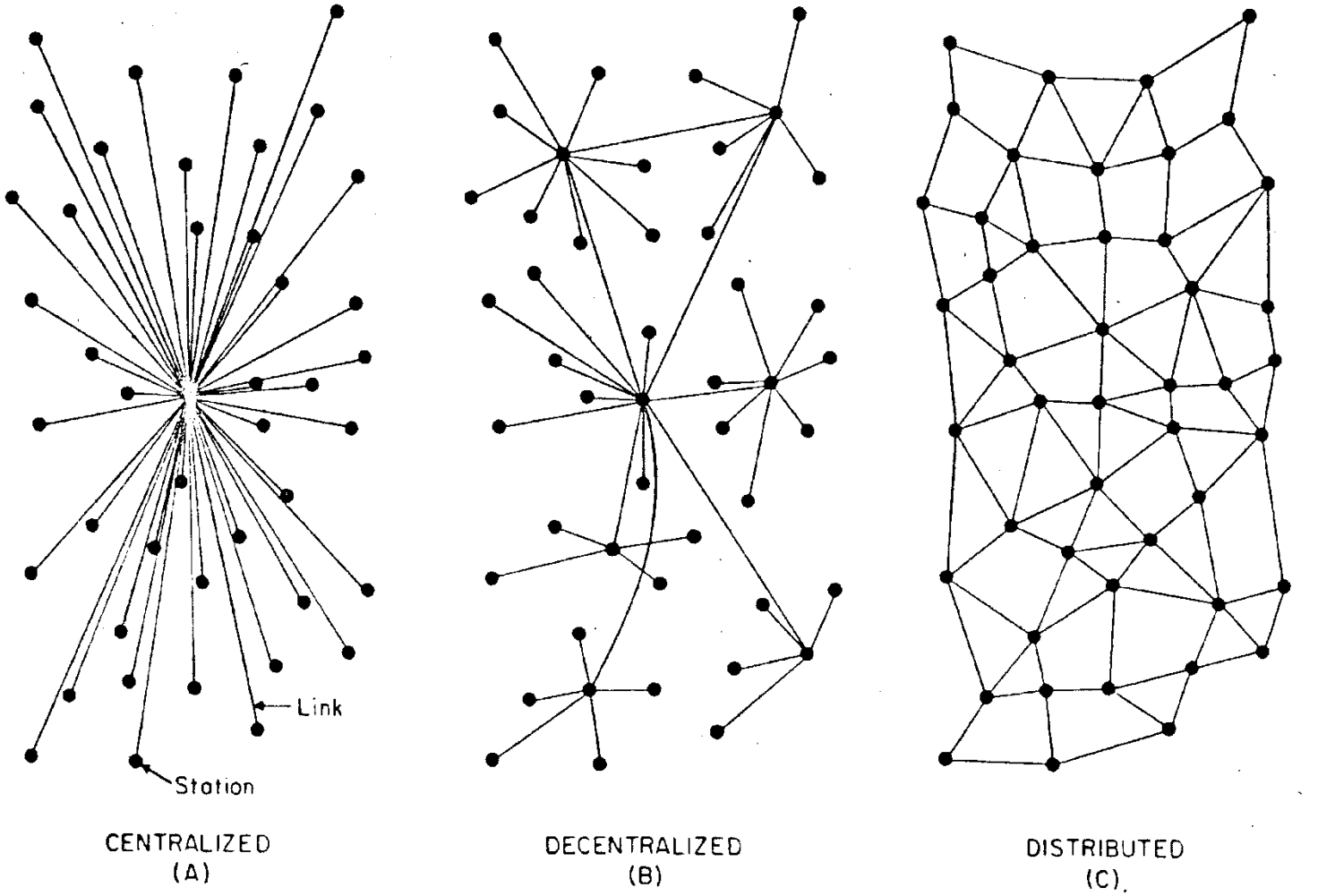
```
from mpi4py import MPI
comm = MPI.COMM_WORLD
size = comm.Get_size()
rank = comm.Get_rank()
name = MPI.Get_processor_name()
if rank == 0:
    print "Rank %d of %d running on %s"
        % (rank, size, name)
    for i in xrange(1, size):
    rank, size, name = comm.recv(source=i, tag=1)
    print “Rank %d of %d running on %s"
        % (rank, size, name)
else:
    comm.send((rank, size, name), dest=0, tag=1)
```



http://pythonhosted.org/mpi4py/
https://software.intel.com/en-us/intel-mpi-library

Distributed Computing

Distributed Computing

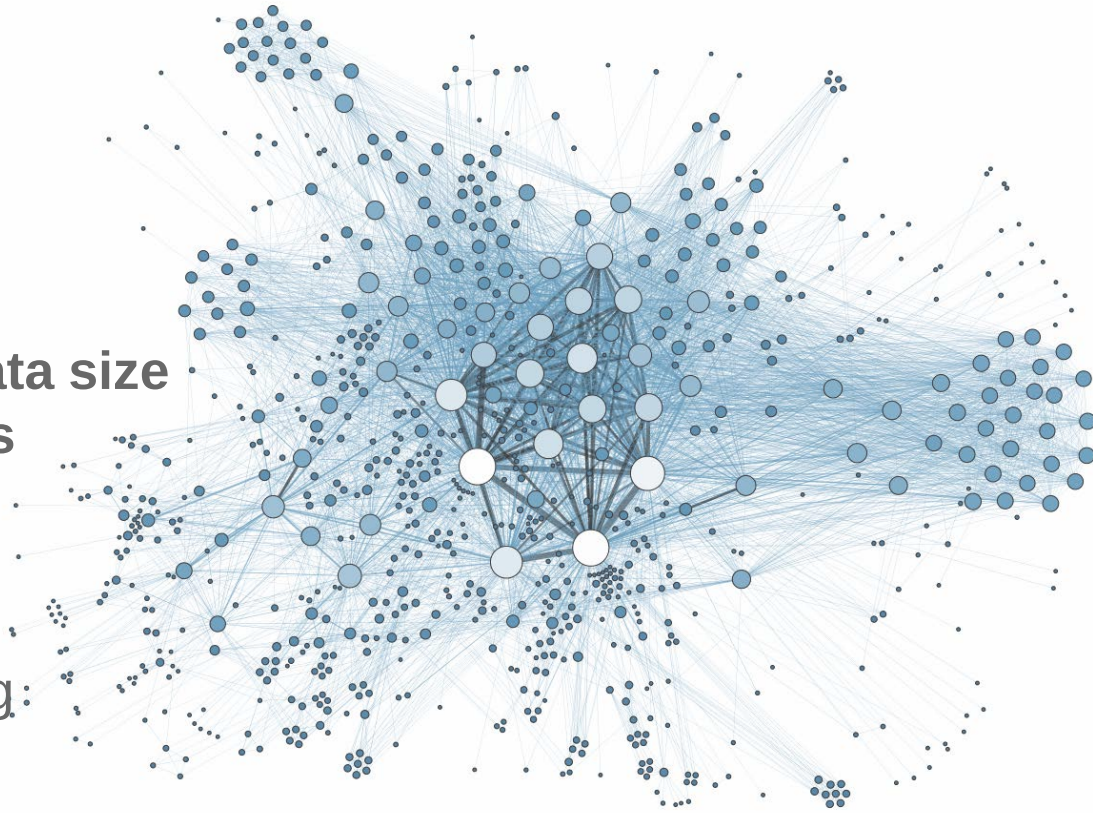


Paul Baran. *On Distributed Communication Networks*. IEEE Transactions on Communications, 12(1):1–9, March 1964

Distributed Computing

Driven by data science, machine learning, predictive analytics, …

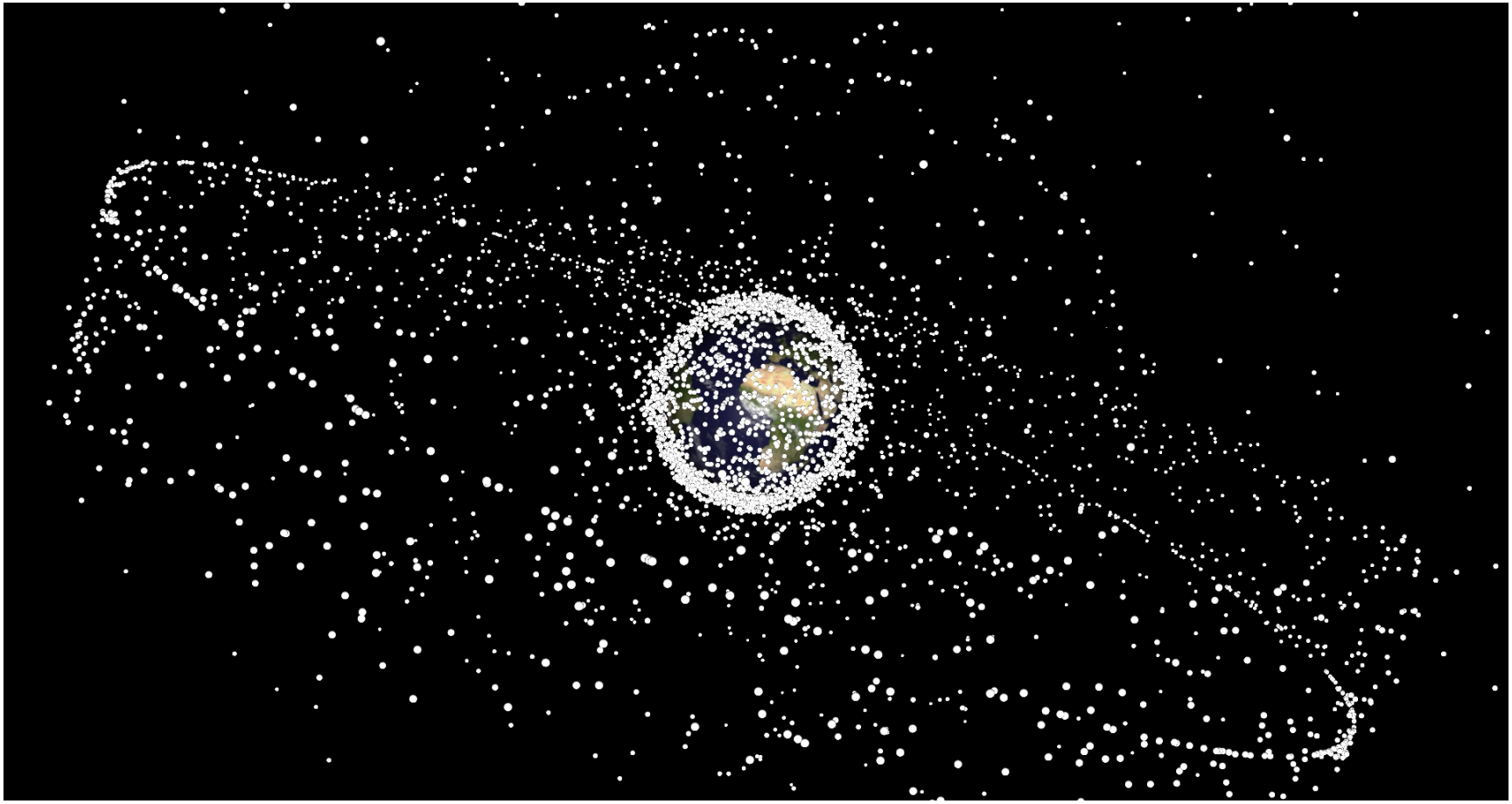
- Tabular data
- Time Series
- Stream data
- Connected data



Scaling up with increased data size from from laptops to clusters

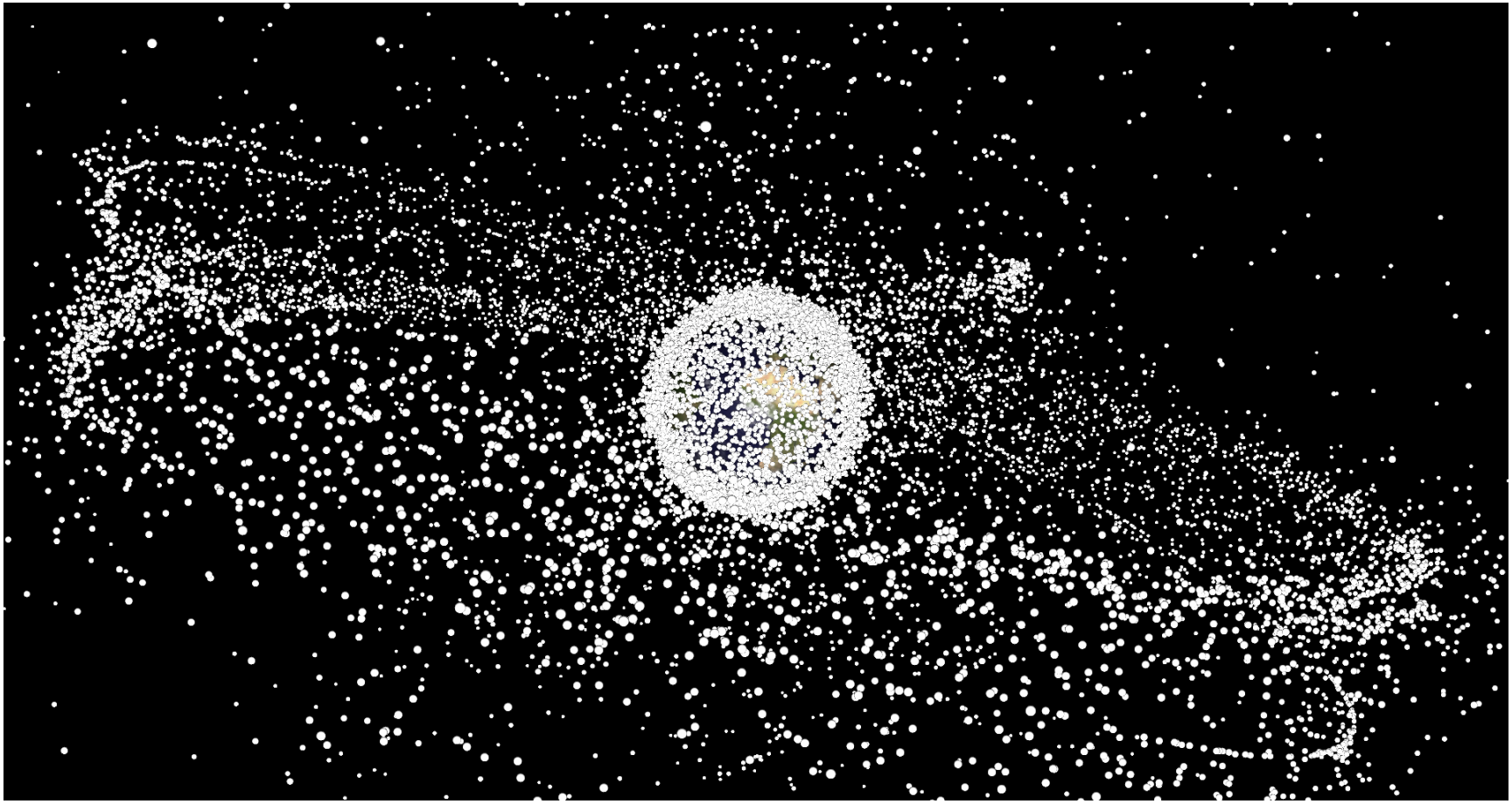
- Many-Task-Computing
- Distributed scheduling
- Peer-to-peer data sharing

Space Debris: Object Correlation from Sensor Data and Real-Time Collision Detection

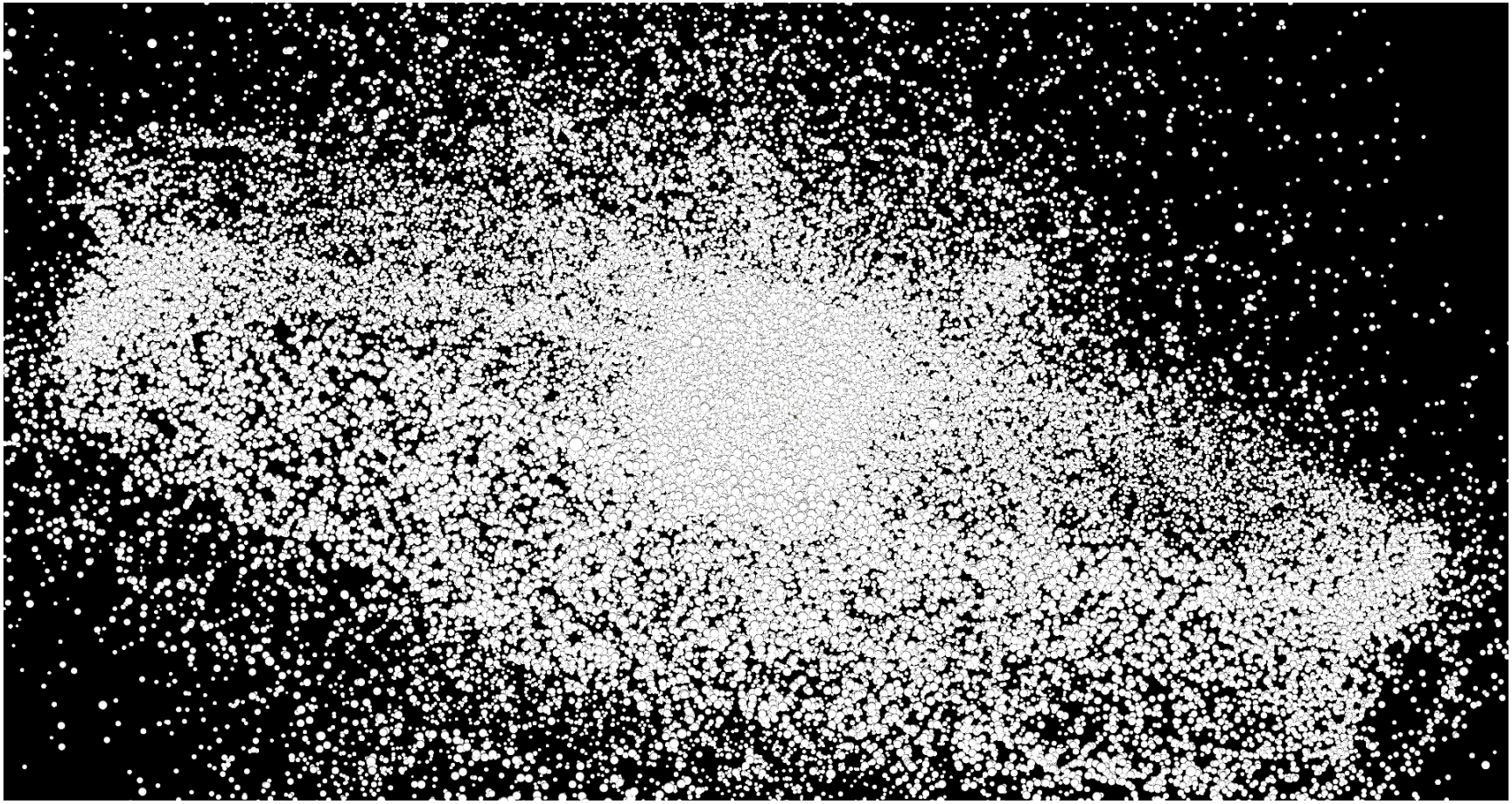


DLR

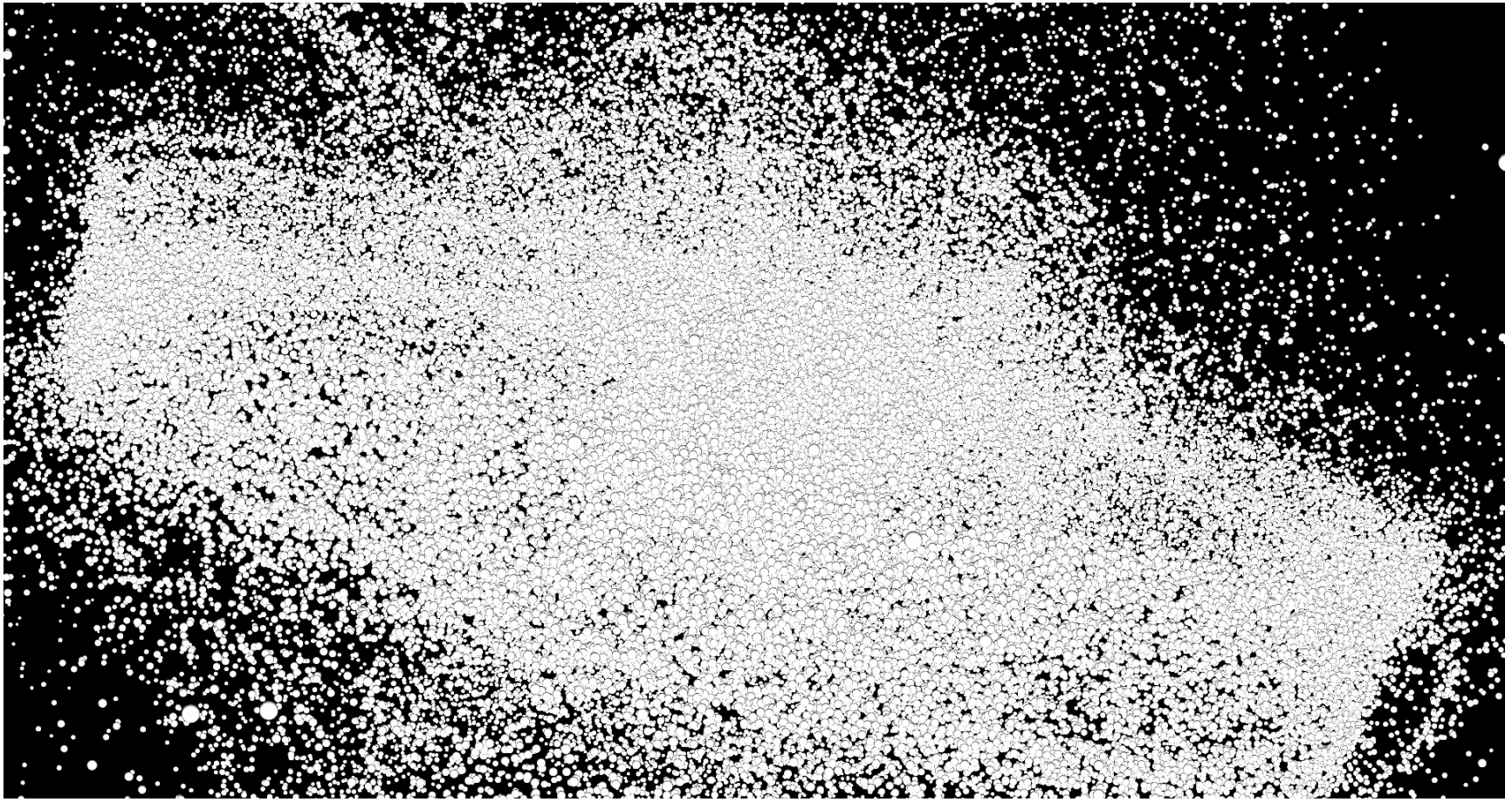
29,000 Objects Larger than 10 cm



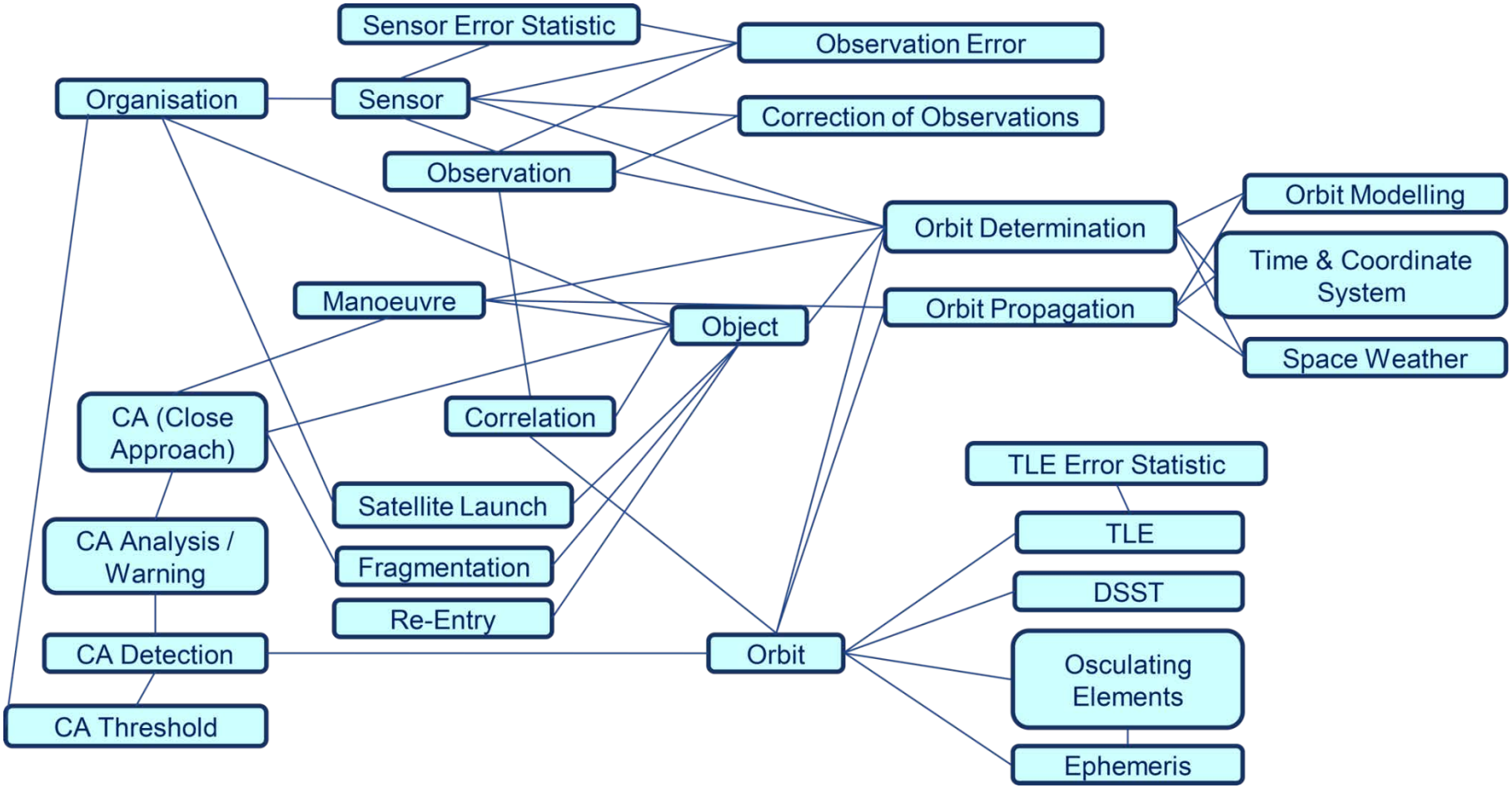
750,000 Objects Larger than 1 cm



150M Objects Larger than 1 mm

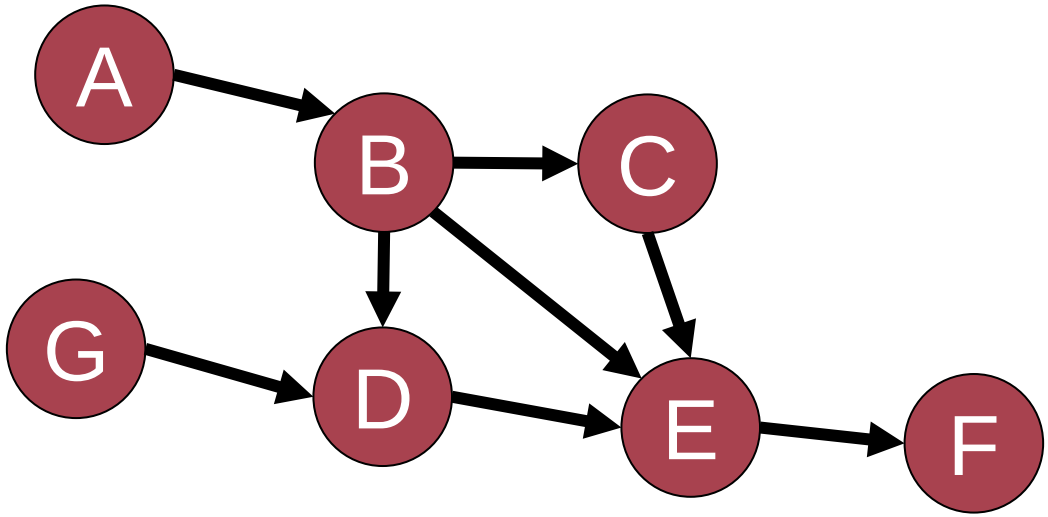


Space Debris: Graph of Computations



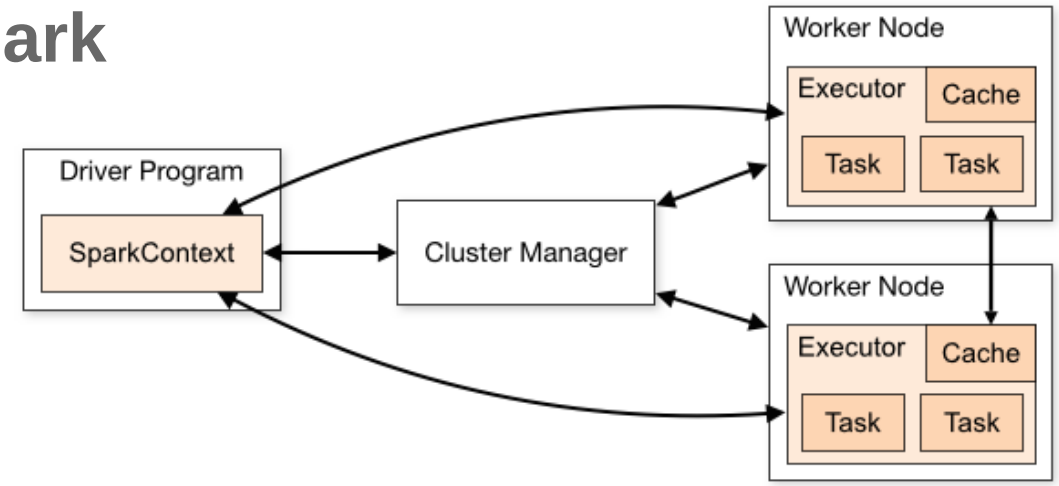
Graphs

Directed Acyclic Graph (DAG)



Python has great tools to execute graphs on distributed resources

PySpark

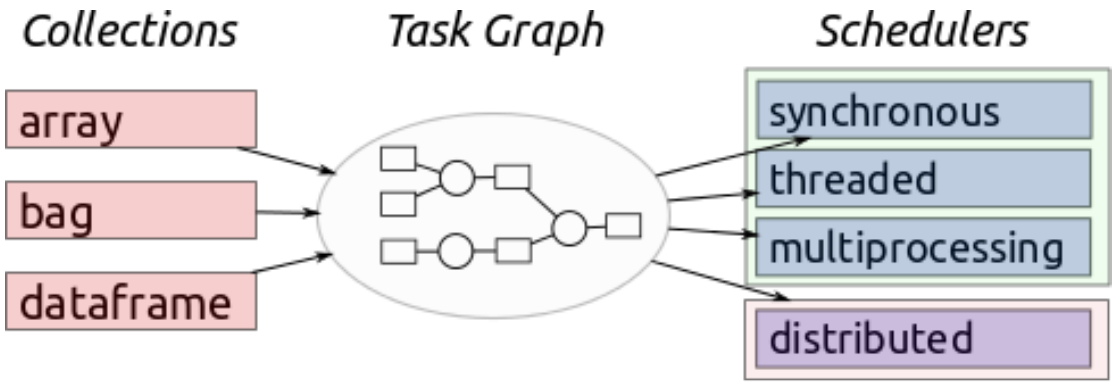



```
from pyspark import SparkContext

logFile = “myfile.txt“
sc = SparkContext("local", "Simple App")
logData = sc.textFile(logFile).cache()

numAs = logData.filter(lambda s: 'a' in s).count()
numBs = logData.filter(lambda s: 'b' in s).count()

print("Lines with a: %i, lines with b: %i" % (numAs, numBs))
```

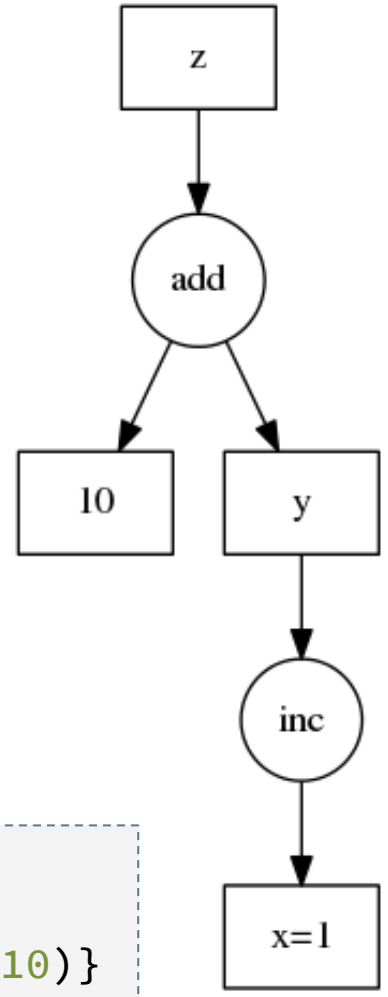
https://spark.apache.org/
https://spark.apache.org/docs/0.9.0/python-programming-guide.html

ANACONDA

Dask




```
import dask.dataframe as dd
df = dd.read_csv('2015-*-*.csv')
df.groupby(df.user_id).value.mean().compute()
```

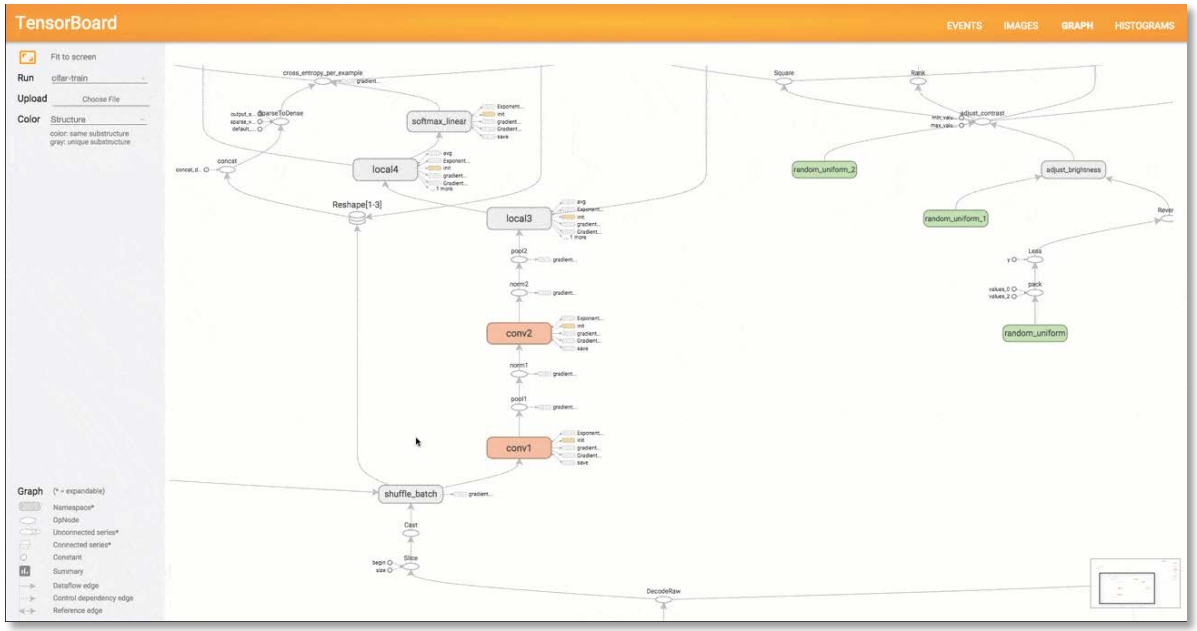



```
d = {'x': 1,
     'y': (inc, 'x'),
     'z': (add, 'y', 10)}
```

http://dask.pydata.org/

DLR

TensorFlow




```
import tensorflow as tf

with tf.Session() as sess:
    with tf.device("/gpu:1"):
      matrix1 = tf.constant([[3., 3.]])
      matrix2 = tf.constant([[2.],[2.]])
      product = tf.matmul(matrix1, matrix2)
```

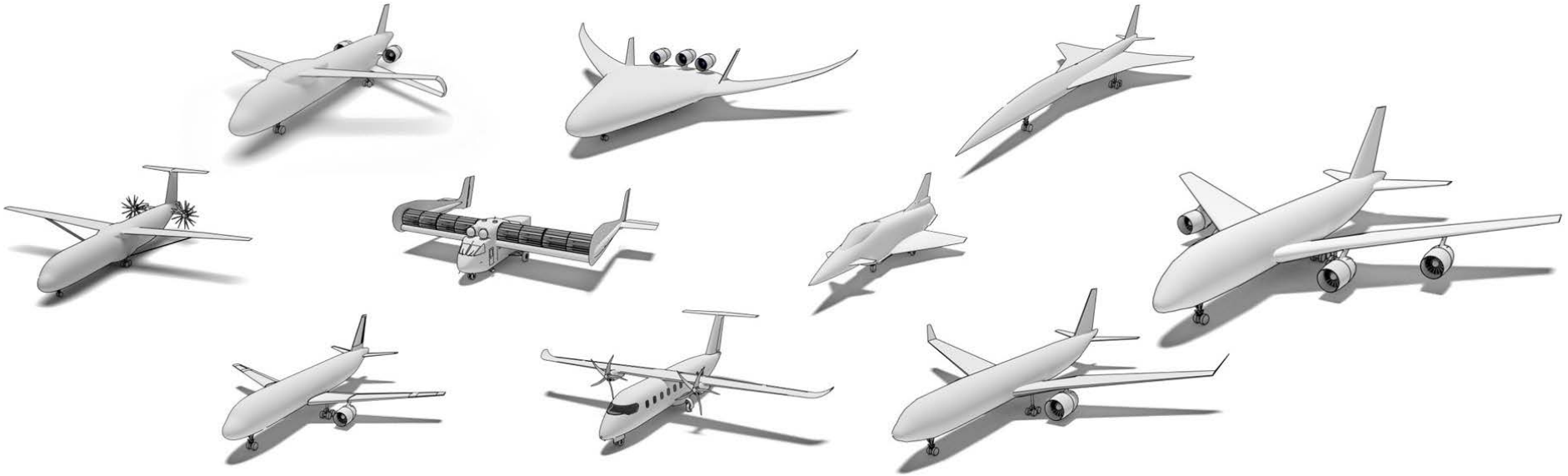
https://www.tensorflow.org/

Quantum Computing

Optimization Problems in Aeronautics & Space

Design optimization and robust design

- Space systems and air transportation systems
- Design and evaluation of systems with consideration of uncertainties



Optimization Problems in Aeronautics & Space

Machine Learning

- Deep learning, pattern recognition, clustering, images recognition, stream reasoning

Anomaly detection

- Monitoring of space systems

Mission planning

- Optimization in relation to time, resource allocation, energy consumption, costs etc.

Verification and validation

- Software, embedded systems

New Research Field: Quantum Computing

Discrete optimization is basis for many kinds of problems

→ Packaging
→ Partitioning
→ Mapping
→ Scheduling

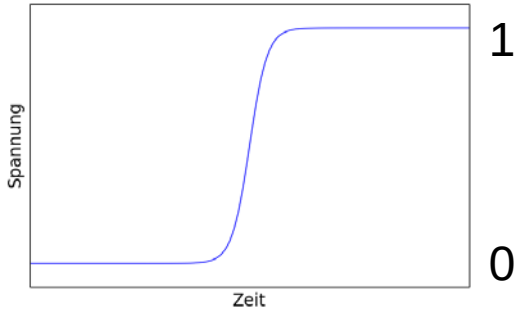
NP-hard problems!

Hope: **Quantum Computers** solve those problems faster than classical computers

Bits and Qubits

Classical Bits

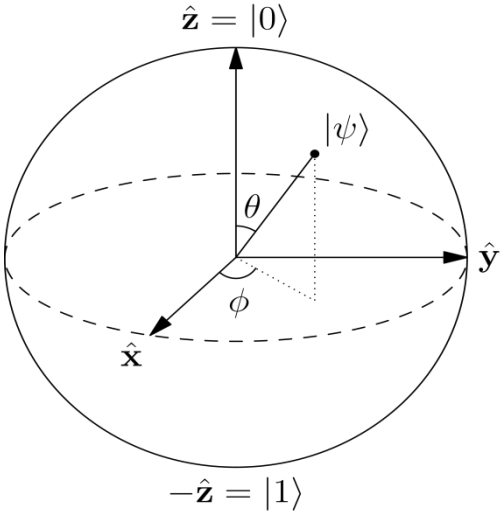
- “0” or “1”
- Electric voltage



Quantum bits (Qubits)

- Superposition of complex base states

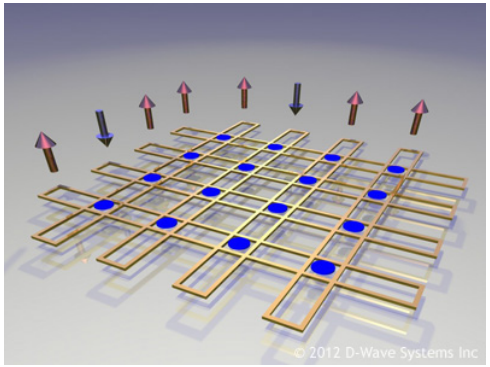
$$|\psi\rangle = c_0|0\rangle + c_1|1\rangle$$



Quantum Computer

To date, one Quantum Computer is available commercially

- D-Wave Systems, Inc., Canada
- System with ~2000 Qubits („D-Wave 2X“)
- Adiabatic QC



Images: © D-Wave Systems, Inc.

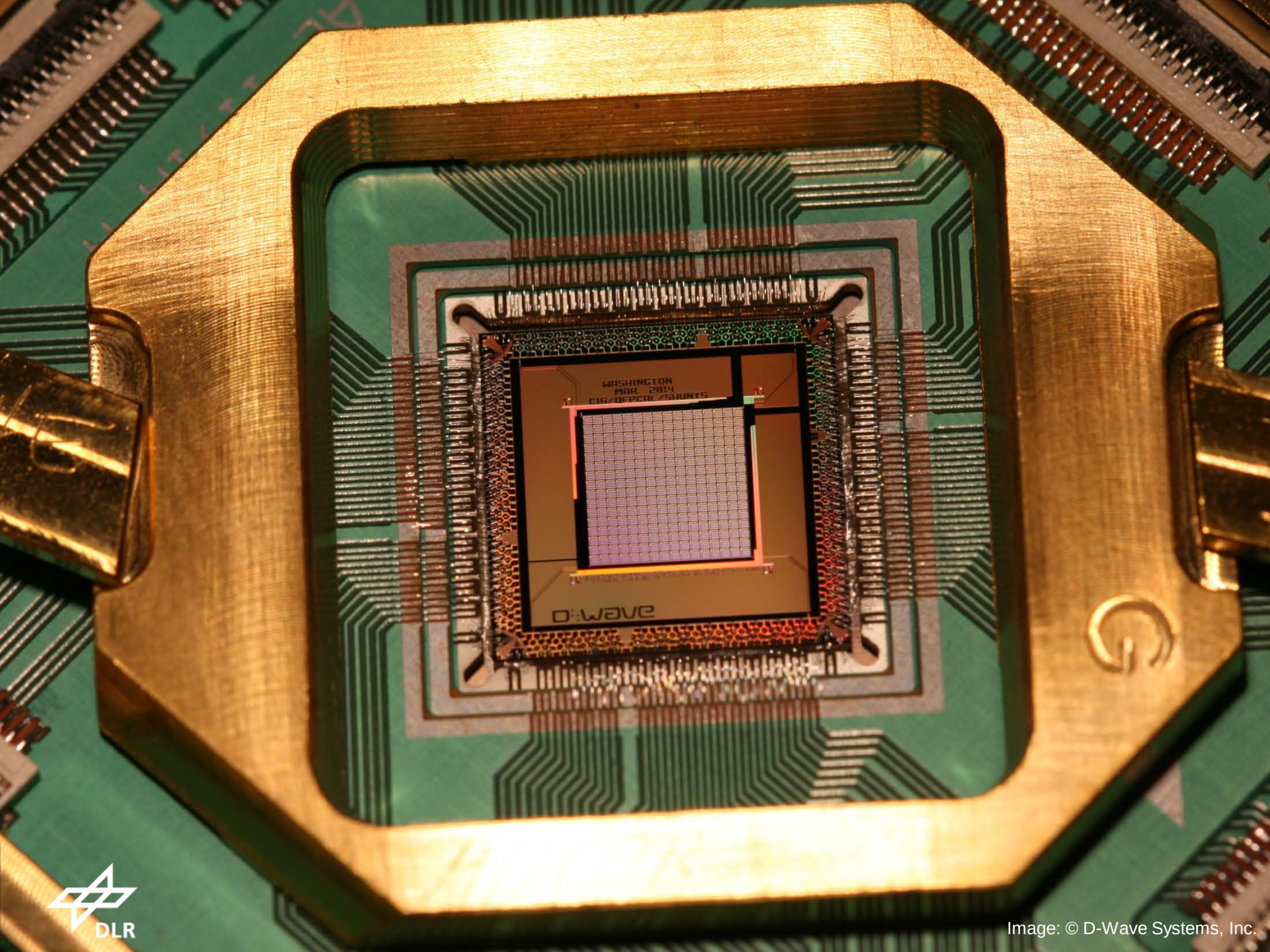


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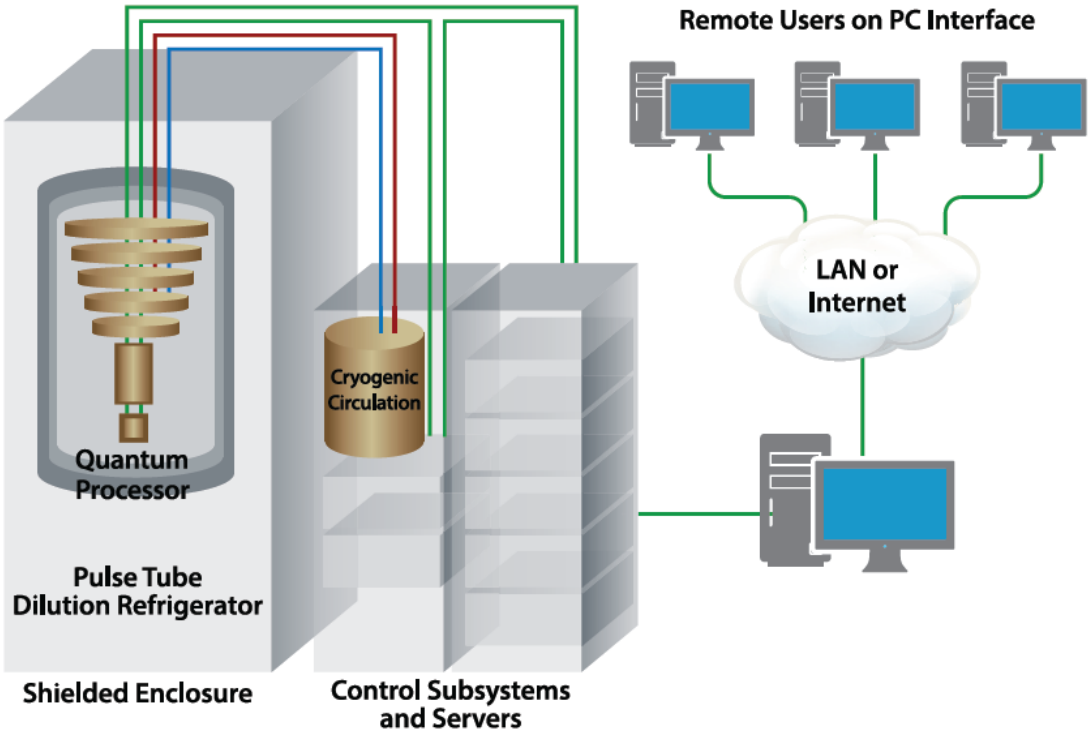
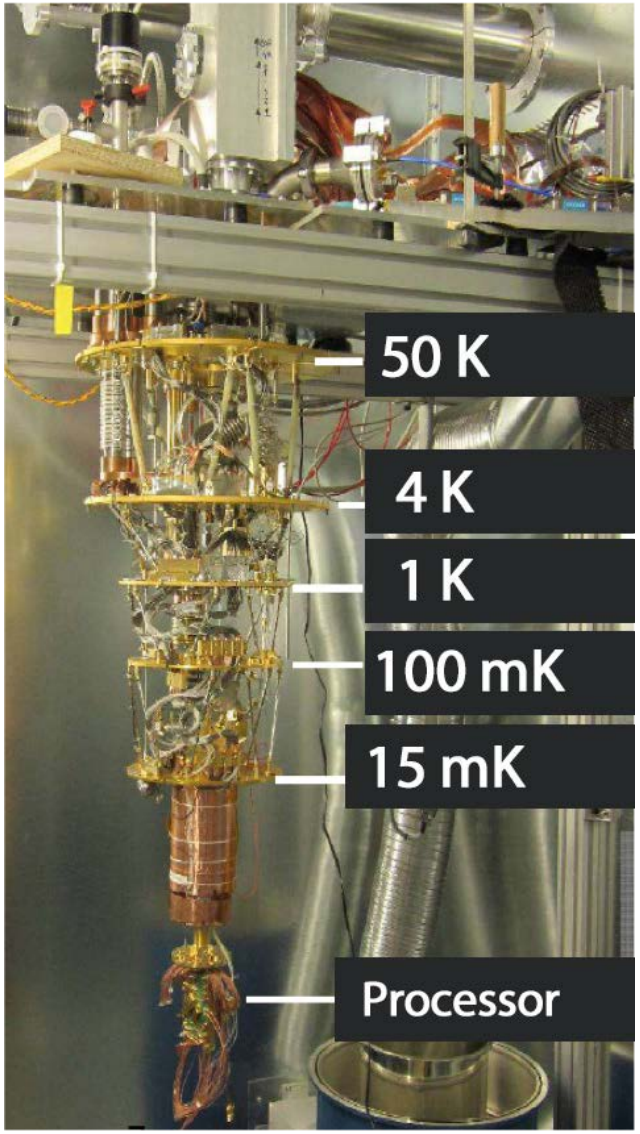
Image: © D-Wave Systems, Inc.

Inside D-Wave 2





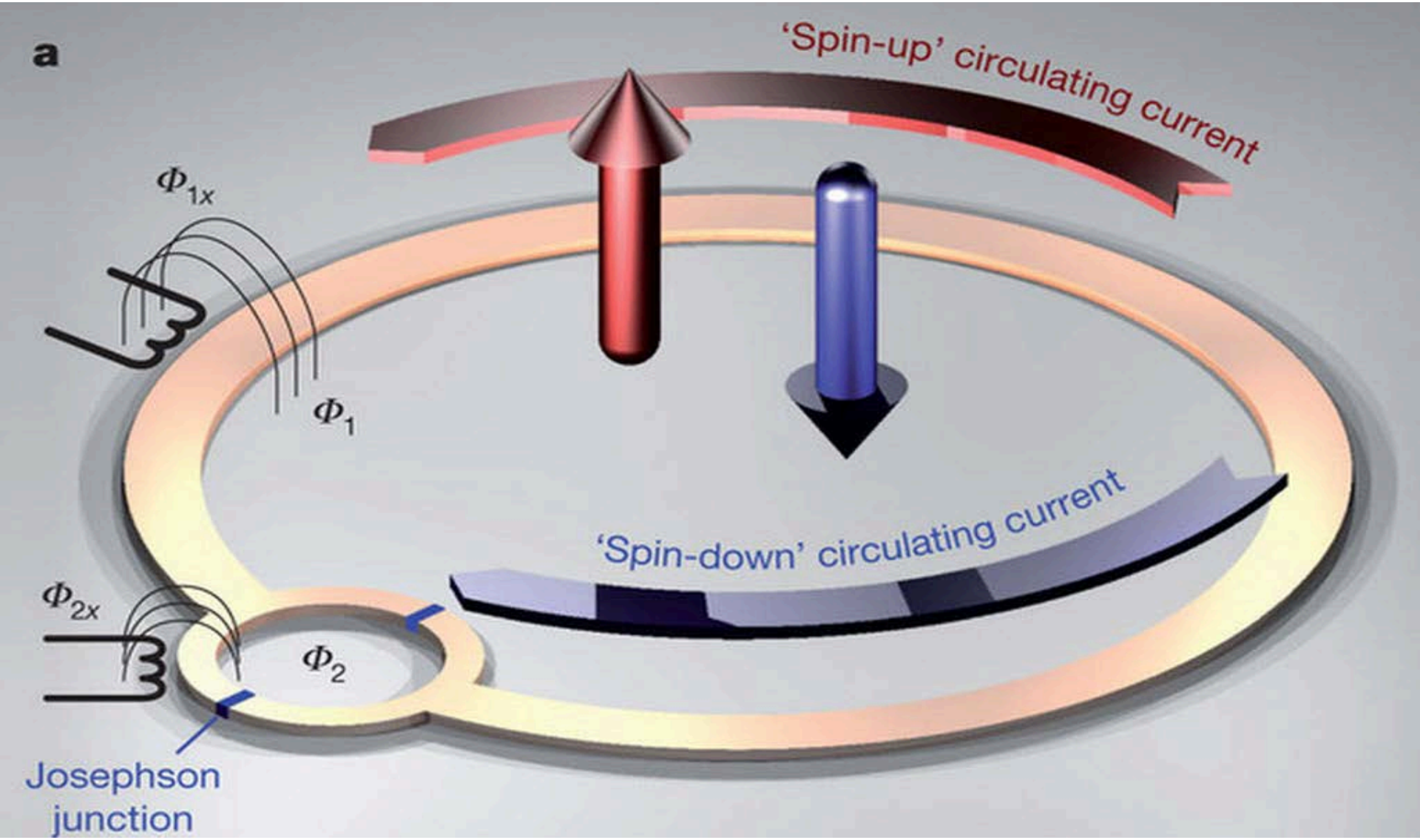
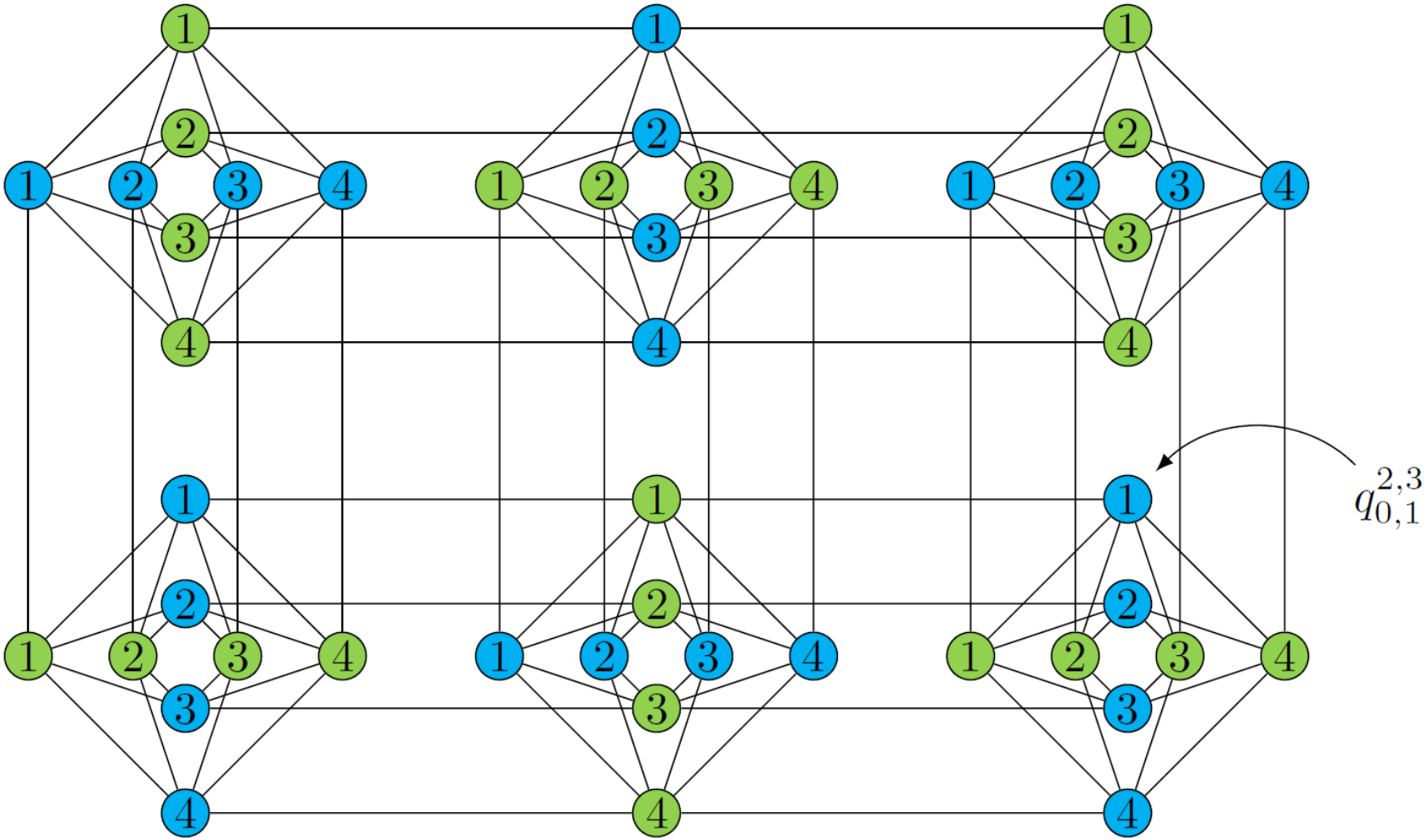


Image: © D-Wave Systems, Inc.

D-Wave Qubit Topology – Chimera Graph



“Programming” a Quantum Computer – Step 1

Rewrite the problem as discrete optimization problem

- **QUBO**: Quadratic unconstrained binary optimization

$$E(q_1, \dots, q_n) = \sum_{i=1}^{n} g_i \, q_i + \sum_{\substack{i,j=1 \\ i>j}}^{n} s_{ij} \, q_i q_j$$

$$q_i = \begin{cases} 0, \text{for switch off} \\ 1, \text{for switch on} \end{cases}$$

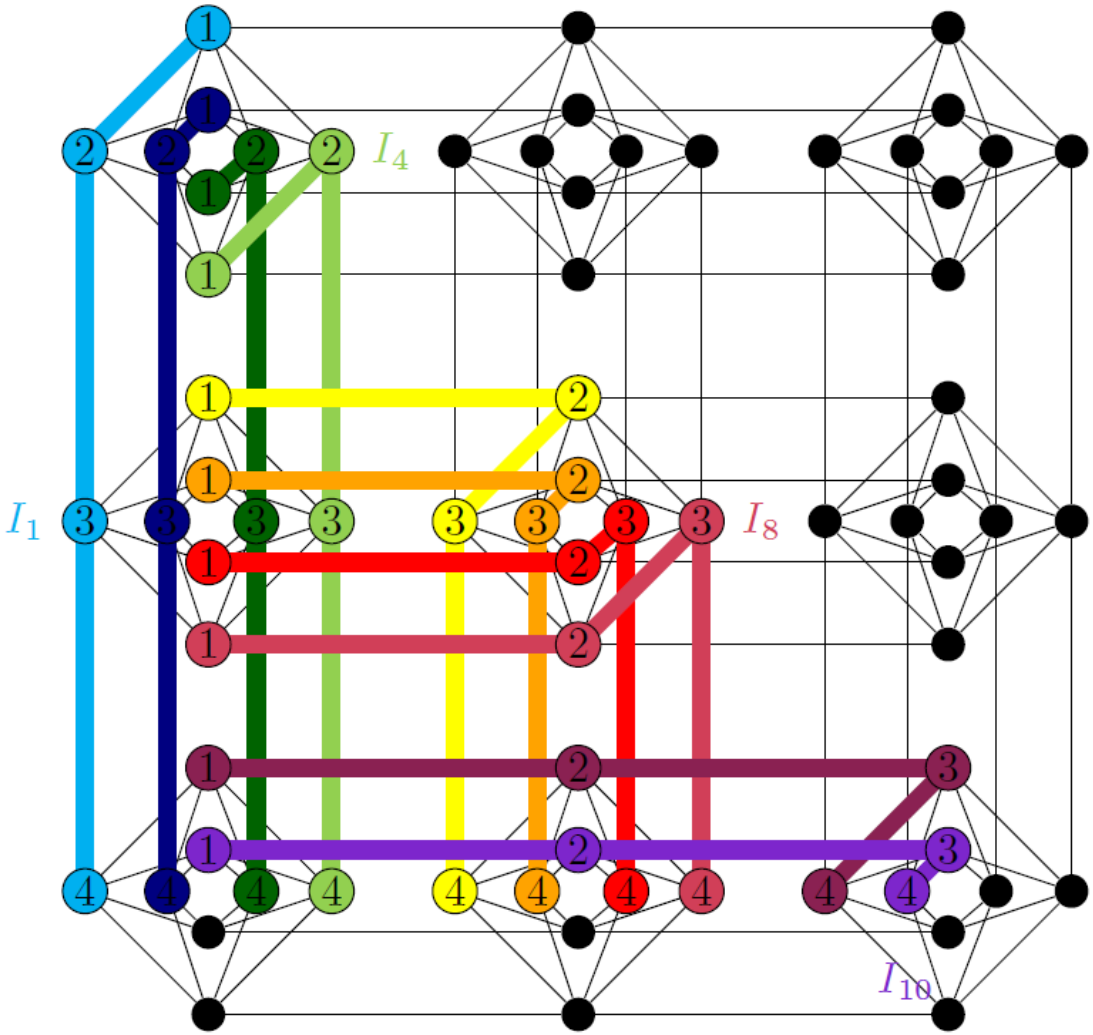
g_i weights

s_{ij} strength of coupling

“Programming” a Quantum Computer – Step 2

Mapping to hardware topology

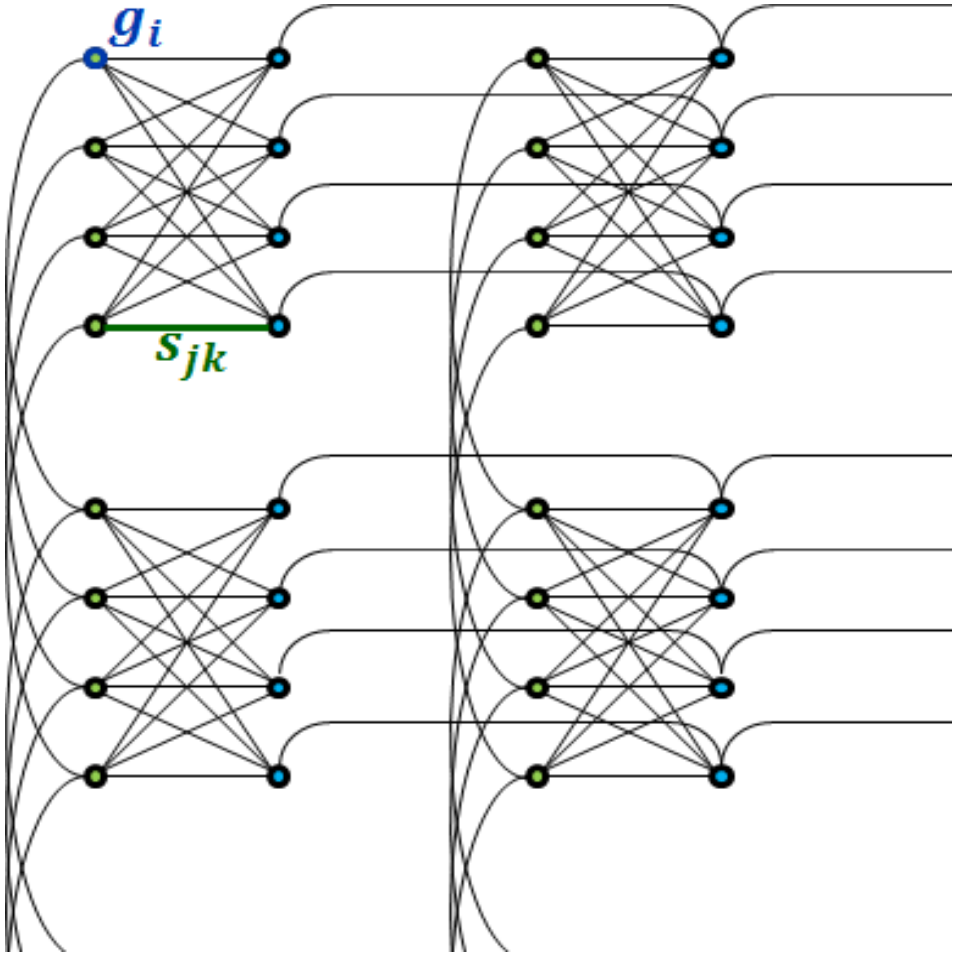
→ Chimera-QUBO



“Programming” a Quantum Computer – Step 3

Bringing the problem to the QC

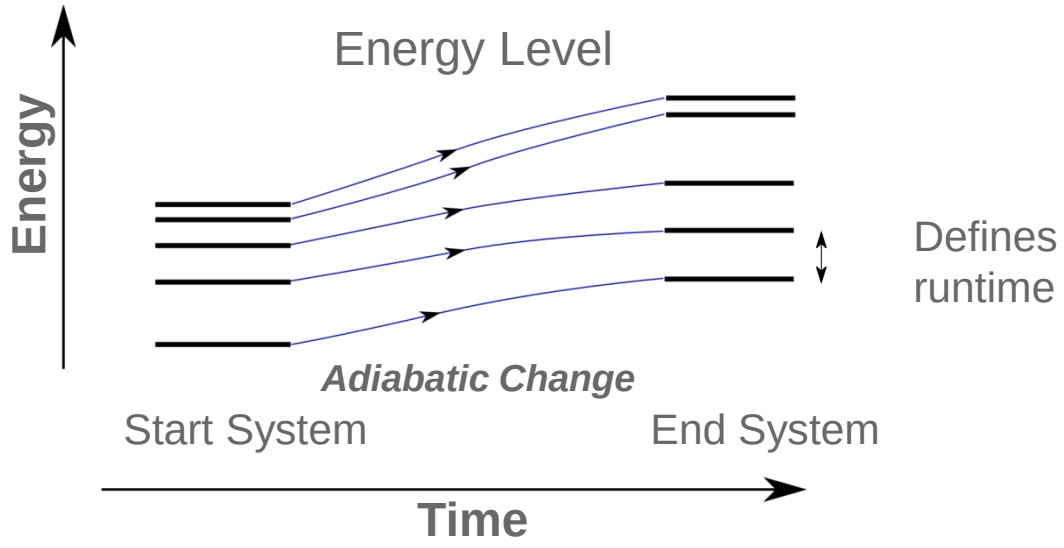
- Copy weights and coupling strengths to physical Qubits



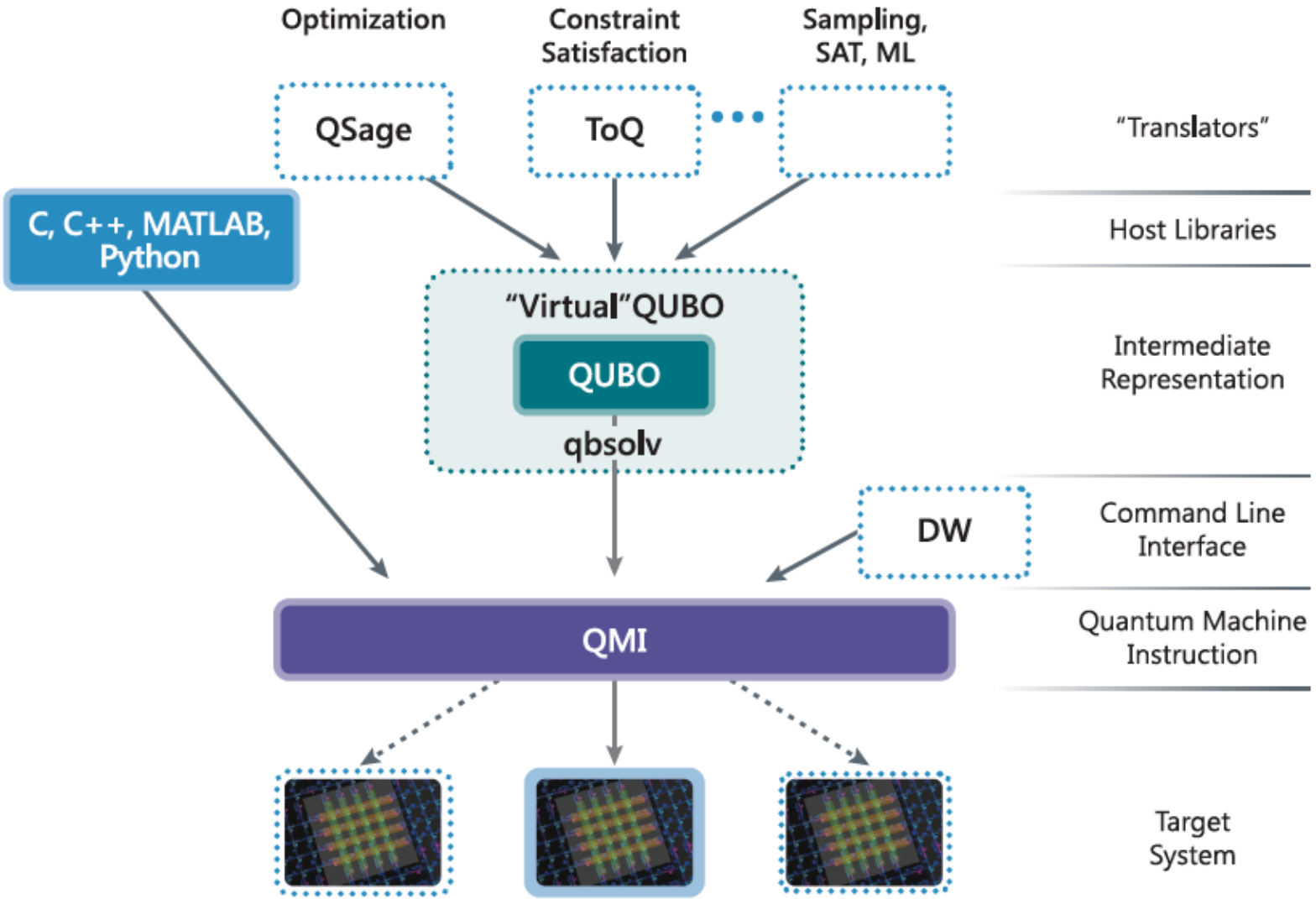
“Programming” a Quantum Computer – Step 4

Starting the actual “computation”:

- Adiabatic process from start energy level to target energy level, which represents solution of the optimization problem
- Result are the voltages after this process



D-Wave Software Environment



Programming with Python

Import API and Connect to Machine

```
import dwave_sapi2.remote as remote
import dwave_sapi2.embedding as embedding
import dwave_sapi2.util as util
import dwave_sapi2.core as core

# print "Connect to DWave machine ..."
# create a remote connection
try:
    conn = remote.RemoteConnection(myToken.myUrl,
                                   myToken.myToken)
    # get the solver
    solver = conn.get_solver('C12')
except:
    print 'Unable to establish connection'
    exit(1)
```

Programming with Python

Prepare the Problem (“Embedding”)

```
hwa = get_hardware_adjacency(solver)


embeddings[eIndex] = embedding.find_embedding(J, hwa)


h_embedded[eIndex], j0, jc, new_embed =
embedding.embed_problem(h, J, embeddings[eIndex], hwa)
J_embedded[eIndex] = jc
J_embedded[eIndex].update(j0)
embeddings[eIndex] = new_embed
```

Programming with Python

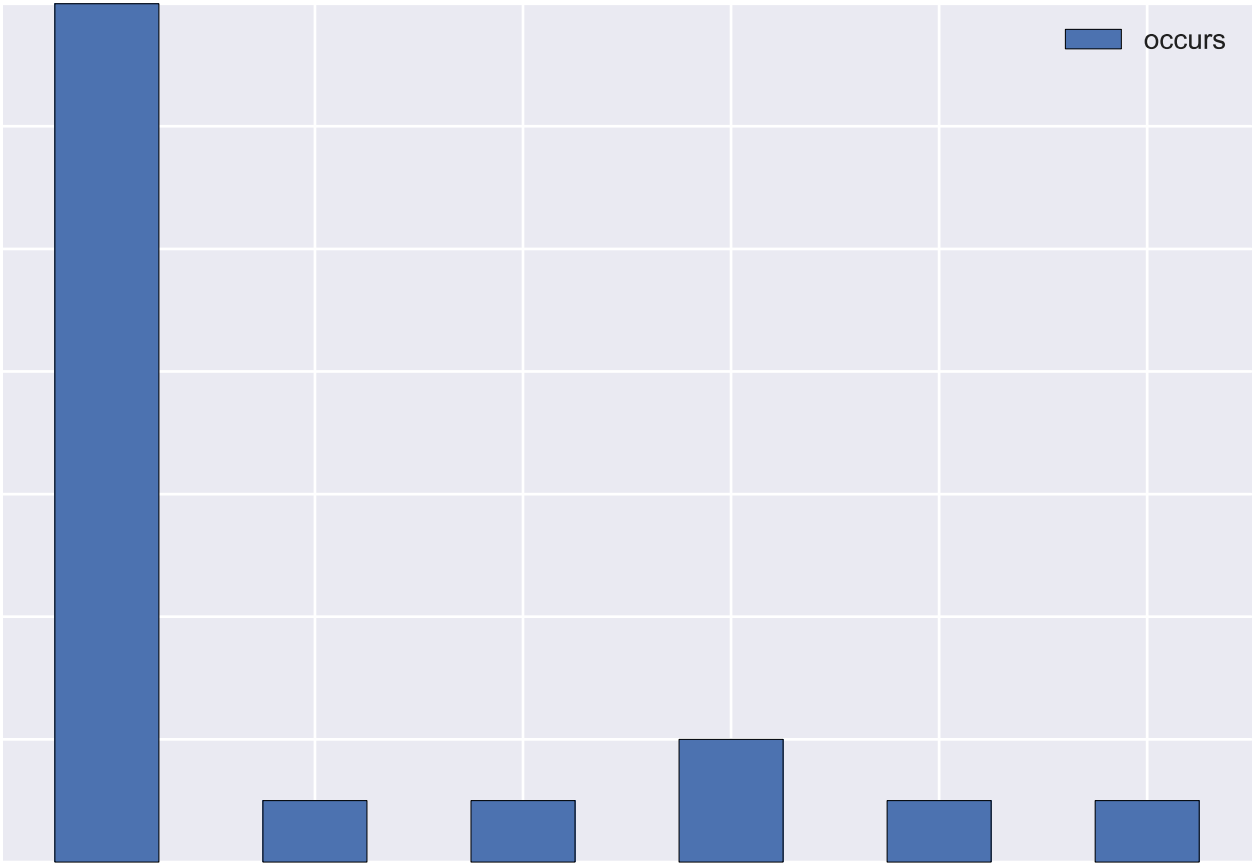
Solve the Problem (“Ising”)

```
getEmbeddedIsing(eIndex)
# print "Annealing ..."
result = core.solve_ising(solver,
                          h_embedded[eIndex],
                          J_embedded[eIndex],
                          annealing_time=20,
                          num_reads=1000)

unembedded_result = embedding.unembed_answer(
                          result['solutions'],
                          embeddings[eIndex],
                          'minimize_energy', h, J)

# take the lowest energy solution
rawsolution_phys = (np.array(result['solutions']) + 1)/2
rawsolution_log = (np.array(unembedded_result) + 1)/2
```

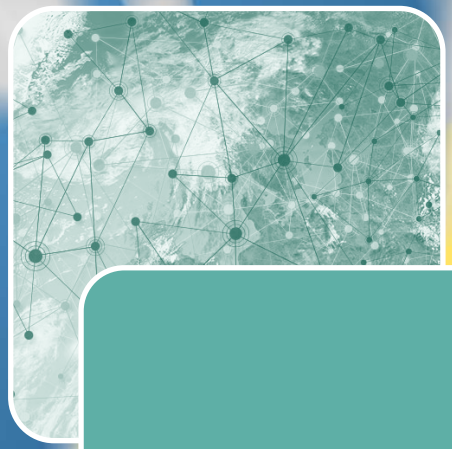
Result Distribution



Summary

Python is or will become standard in programming for...

High Performance



Data Science

Future Architectures

Thank You!

Questions?

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